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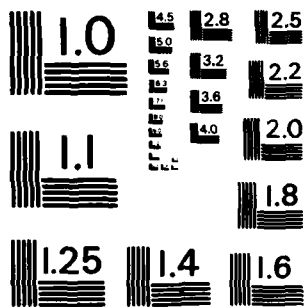
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ATR CODE IMPROVEMENTS

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SECTION 1

INTRODUCTION

This document describes some modifications to the ATR code which improve the prediction of delayed radiation dose by incorporating the variation in fission product source strength with the fissioning isotope concentrations, permit the user more flexibility in specifying the air density, and incorporate additional user convenience commands.

The delayed radiation modification task was commenced on the recommendation of Jess Marcum (Reference 1). During the course of this effort, whose modest scope was to change only the source output normalization for each fission isotope (^{235}U , ^{238}U , ^{239}Pu) and to add commands to permit specification of relative concentration of each isotope, interest developed to advance the state-of-the-art of delayed radiation phenomenology by analyzing in detail the time energy-dependent variation of the fission product sources from each isotope as well as the hydrodynamic enhancement effects, fireball rise, and spatial distribution of sources within the fireball. Consequently, a more comprehensive analysis was conducted as a separate research project. The current ATR code (ATR/ISO) with the improved delayed radiation module reflecting this more ambitious scope of work is reported in a separate document (Reference 2).

The additional user convenience commands were added at the request of the U.S. Army Nuclear and Chemical Agency (USANCA) in memo to Dr. David Auton in September 1979. These additional commands are described in Section 2 of this report.

The air density variation with altitude in ATR was based on the U.S. Standard Atmosphere (USSA) and did not permit modifications for temperature variation and the effects of ground on the temperature variation. Thus the air density, at say, 6 Kft above sea level was the same for a ground elevation of 500 feet or 5 Kft above sea level. In principal, an ATR user could obtain the correct ground correction factors and air mass penetration from source to target, but the procedure was very cumbersome. A revised air

density model was added with some new commands during the course of this effort which facilitates the detailed specification of the atmosphere for ATR calculations. This is described in Section 3 of this report.

Pending more substantive modifications to the ATR code which materially effect the results output to user, the changes described here will not be released to avoid proliferation of versions of the code.

SECTION 2

ATR COMMAND MODIFICATIONS AND ADDITIONS

Because of the wider acceptance by the community of tissue kerma as a more relevant neutron dose response than the Henderson tissue dose response, the computation of total tissue dose which sums the neutron and various gamma-ray components will now use tissue kerma for the neutron component replacing the previously used Henderson tissue dose (Reference 3).

An new command sequence has been added to allow the user a choice of ground correction factors. This sequence is

- *CORF = Turn "off" correction factors, that is, no ground corrections are applied.
- *CORL = Use "old" correction factors. That is, use the correction factors embodied in ATR Version 4 as described in Reference 3. These are based on calculations by Pace (Reference 4).
- *CORN = Use "new" correction factors. That is, use the correction factors in ATR Version 4.1 described in Reference 5. These are based on calculations by Gritzner and Straker embodied in TWEEDDEE Code (Reference 6).

The term "old" and "new" reflect a chronological artifact and do not imply quality distinctions. The default command is CORN. Use of the above commands sets a switch for the requested correction factors which remain in effect until superseded by another command in the sequence.

A new command has been added to allow the user to specify dose transmission factors for individual dose components. The command is:

*TRAN/X/f

where X = N for neutrons, NG for secondary gamma rays, G for prompt gamma-rays, and FP for fission product gamma-rays; and f = the dose transmission factor. The factor is applied to all dose calculations and is operative in

the application of *CONSTRAINT command. The default value is $f = 1$. The command remains in effect until superseded or a

*DEL TRAN

command is given.

SECTION 3

MODIFICATION TO ATR FOR ALTITUDE SPECIFICATION

The objective of this modification is to permit the ATR user to specify the air density and density gradient needed by ATR with greater flexibility. The basic default atmosphere is pegged to U.S. Standard Atmosphere (USSA) used in previous versions.

The air density is governed by the gas equation:

$$P = \rho \frac{RT}{M} \quad (1)$$

where p = air pressure (newton/m² = 0.01 millibar)

ρ = density (kg/m³)

R = universal gas constant $\left(8.31432 \times 10^3 \frac{\text{newton m}}{\text{kmol } ^\circ\text{K}} \right)$

T = temperature (^oK)

M_o = average molecular weight $\left(28.9644 \frac{\text{kg}}{\text{kmol}} \right)$

The molecular weight varies with humidity and with altitude above 86 km. A molecular temperature T^* is defined so that:

$$T^* = 28.9644 \frac{T}{M} \quad (2)$$

which facilitates treatment of varying molecular weight.

The hydrostatic equation governs the altitude pressure variation.

It is:

$$dP = -\rho g dZ \quad (3)$$

where g = gravity acceleration $g(Z=0) = 9.80665 \text{ m/sec}^2$

Z = geometric altitude (m)

A geopotential altitude H is defined as:

$$g_0 dH = g dZ \quad (4)$$

so that the variation of gravity can be eliminated. Since the variation of gravity with respect to Z is:

$$g = g_0 \left(\frac{r_0}{r_0 + Z} \right)^2 \quad (5)$$

where $r_0 = 6.356766$ m, H is related to Z by

$$H = \frac{r_0 Z}{r_0 + Z} \quad \text{or} \quad Z = \frac{r_0 H}{r_0 - H} \quad (6)$$

Before the gas equation (1) and the hydrostatic equation (3) can be solved, the temperature dependence with altitude must be assumed. The U.S. Standard Atmosphere provides a temperature model linear with geopotential over seven regions up to 86 km. Thus

$$T^* = T_i^* + L_i (H - H_i) \quad H_i < H < H_{i+1} \quad (7)$$

for seven regions given the table below.

i	H_i (km)	L_i (°K/km)	T_i °K	P_i (mbar)
1	0 and below	-6.5	288.15	1.01325+3
2	11	0.0	216.65	2.2632+2
3	20	1.0	216.65	5.4748+1
4	32	2.8	228.65	8.6801+0
5	47	0.0	270.65	1.1090+0
6	51	-2.8	270.65	6.6938-1
7	71	-2.0	214.65	3.9564-2
	84.5		187.65	3.9814-2

Now equations (1), (3), and (7) can be solved for the pressure by eliminating density

$$\frac{dP}{P} = -g_0 \frac{M_0 dH}{R[T_i^* + L_i(H - H_i)]} \quad (8)$$

There are two solutions to this equation depending on whether or not L_i is zero. Normally L_i is not zero and

$$p(H) = \frac{P_i M_0}{R T_i^*} \left[\frac{T_i^*}{T_i^* + L_i(H - H_i)} \right] \left(\frac{g_0 M_0 \times 10^3}{R L_i} + 1 \right) \quad (9)$$

When L_i is zero the solution is the exponential atmosphere:

$$p(H) = \frac{P_i M_0}{R T_i^*} \exp \left[\frac{-g_0 M_0 (H - H_i) \times 10^3}{R T_i^*} \right] \quad (10)$$

Equations (9) and (10) define the U.S. Standard Atmosphere. The P_i (pressures at the seven boundary layers) are calculated from the bottom to the top by setting $P_1 = 1.01325(+3)$ mbar and calculating P_{i+1} for H_{i+1} in either (9) and (10). This treatment is valid below 85 km.

The default atmosphere in ATR is the U.S. Standard Atmosphere, but the user can now modify it with the new command structure by specifying other conditions at a single altitude, or the user can force a density profile on a single altitude band within this standard atmosphere by inputting pairs of altitude and density values.

The single point altitude change commands are:

- *ELEV/UNIT/HP - specification elevation - single point where user will specify modifications to the USSA. Default value of HP is ground elevation. UNIT = M, FT, KM, KFT, MI, default is meters.
- *TEMP/UNIT/TP - temperature at HP. Default is calculated from input PP and DP or 15°C. Unit = C (°C), K (°K), or F (°K), default is °C.
- *PRES/UNIT/PP - pressure at HP. Default is calculated from input TP and PP or USSA value at HP. UNIT = MB (millibar), TR (torr), HG (in Mercury), PSI (lbs/in²), LBF (lbs/ft³), default is MB.
- *DENSE/UNIT/DP - density at HP. Default is calculated from TP and PP. UNIT = KGM (Kg/m³), GMC (gm/cm²), LBF (lbs/ft³) default is GMC.

NOTE: An input DP and TP will over ride an input PP.

The single point modification of USSA is performed in the following way.

Equation (1) defines a triplet between TP, PP, and DP at altitude HP. If all three are specified, only TP and DP are used and the input value of PP is ignored. If any two are input, the third is calculated from equation (1). If none or only one are specified, the default values are

TP = 15°C

PP = USSA value from equations (9) or (10)

DP = calculated from equation (1) and TP, PP values.

This defines the atmosphere only at HP.

Define the geopotential altitude HG by:

$$HG = \frac{r_0 HP}{r_0 + HP} \quad (11)$$

and to calculate the rest of the atmosphere, if needed, the values of T_i and P_i (Table 1) nearest to the altitude nearest HG are adjusted. This requires adjusting two L_i 's so that the temperature dependence is continuous. In the lowest altitude band we only change L_1 . The procedure for modifying T_i , L_i , and L_{i+1} is illustrated in Figure 1 for two examples. The figure presents the USSA temperature vs. geopotential altitude.

First consider a user specifying a point P_1 in Figure 1 corresponding to values HG, TP, PP, and DP. HG is closer to H_1 than H_2 . Therefore T_1 , P_1 , and L_1 will be modified by linear interpolation

$$T'_1 = T_2 - \frac{H_2 - HG}{H_2 - H_1} (T_2 - TP)$$

$$L'_1 = \frac{T_2 - T'_1}{H_2 - H_1}$$

P'_1 must be calculated from equation (9) (use equation (10) if $L'_1 = 0$), via

$$P'_1 = PP \left[\frac{TP}{TP + L'_1 (H_1 - HG)} \right] \left(\frac{g_0 M_0}{R L'_1} \right)$$

Now with P_1 , T_1 , and L_1 redefined to P'_1 , T'_1 , and L'_1 equation (9) or (10) can be used to get any density.

In the second case in Figure 1 the user specified altitude which is not near the ground. The procedure is similar except that T_4 , P_4 , L_3 , and L_4 must be modified in order to assure temperature continuity. Here

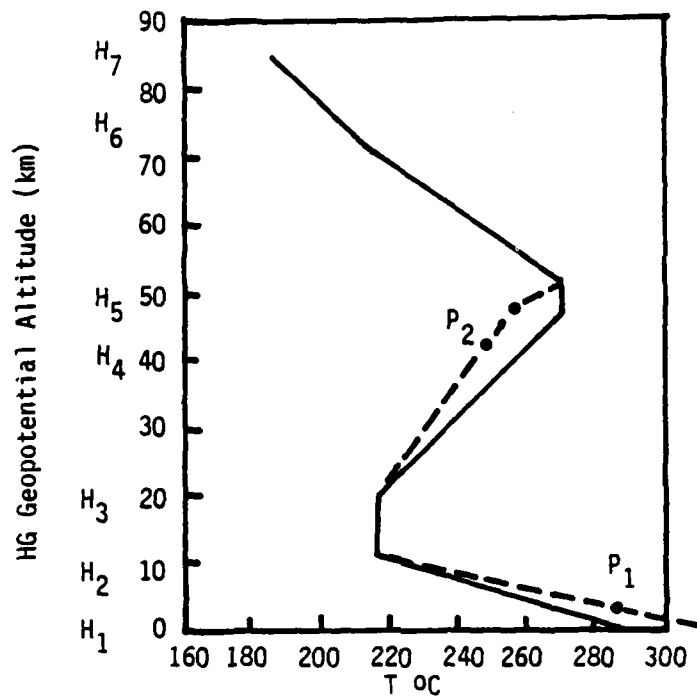


Figure 1. USSA temperature vs. geopotential (solid line). Two examples of user modifications shown as dotted lines.

$$T_4' = T_3 + \frac{HG - H_3}{H_4 - H_3} (TP - T_3)$$

and

$$L_3' = \frac{T_4' - T_3}{H_4 - H_3}$$

and

$$L_4' = \frac{T_5 - T_4'}{H_5 - H_4}$$

and finally,

$$P_4' = PP \left[\frac{TP}{TP + L_3' (H_4 - HG)} \right] \left(\frac{g_o M_o}{R L_3'} \right)$$

Now we can specify the general case procedure. First we calculate $HG = \frac{r_o HP}{r_o + HP}$ and test HG against H_i to get i . Then we test whether HG is above or below the midpoint of that i :

if $HG < (H_i + H_{i+1})/2$, we modify T_i , P_i , L_i , and L_{i-1} ;

if $HG \geq (H_i + H_{i+1})/2$, we modify T_{i+1} , P_{i+1} , and L_{i+1} .

Now, if $HG < (H_i + H_{i+1})/2$, we have

$$T_i = T_{i+1} - \frac{H_{i+1} - HG}{H_{i+1} - H_i} (T_{i+1} - TP)$$

and

$$L'_{i-1} = \frac{T'_i - T_{i-1}}{H_i - H_{i-1}} \quad (\text{not needed if } i = 1)$$

and

$$P'_i = PP \left[\frac{TP}{TP + L'_i (H_i - HG)} \right] \left(\frac{g_o M_o}{R L'_i} \right)$$

However, if $HG \geq (H_i + H_{i+1})/2$, we have

$$T'_{i+1} = T_i + \frac{HT - T_i}{H_{i+1} - H_i} (TP - T_i)$$

and

$$L'_i = \frac{T'_{i+2} - T_i}{H_{i+1} - H_i}$$

and

$$L'_{i+1} = \frac{T_{i+2} - T'_{i+1}}{H_{i+2} - H_{i+1}} \quad (\text{not needed if } i = 6)$$

and

$$P'_{i+1} = PP \left[\frac{TP}{TP + L'_i (H_{i+1} - HG)} \right] \left(\frac{g_o M_o}{T L'_i} \right)$$

If the user wishes to over ride the density profile, the commands are:

ALT/UNIT/HR₁ HR₂.... - array of altitudes to specify a density profile, no default. Units same as ELEV command.

$$HR_i < HR_{i+1}.$$

RHO/UNIT/HD₁ HD₂.... - array of densities corresponding to HR, no default. Units are same as DENSE command.

When the ATR user inputs pairs of (HR_i, DR_i) to specify his own density profile, these override the previous atmosphere in the range included in HR₁ to HR_N. Interpolation between HR_i and HR_{i+1} assumes an exponential atmosphere and is performed by

$$\rho(Z) = \rho_i \left[\frac{\rho_{i+1}}{\rho_i} \right]^{\left(\frac{Z - HR_i}{HR_{i+1} - HR_i} \right)}$$

However if $\left| \frac{\rho_{i+1} - \rho_i}{\rho_i} \right| < 0.001$ linear interpolation is used via

$$\rho(Z) = \rho_i + \frac{(\rho_{i+1} - \rho_i)}{(HR_{i+1} - HR_i)} (Z - HR_i)$$

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